# Predicting the critical density of topological defects in $O(N)$ scalar field theories.

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$O(N)$ symmetric $\lambda\phi^4$ field theories describe many critical phenomena in the laboratory and in the early Universe. Given $N$ and $D \leq 3$, the dimension of space, these models exhibit topological defect classical solutions that in some cases fully determine their critical behavior. For $N = 2$, $D = 3$ it has been observed that the defect density is seemingly a universal quantity at $T_c$. We prove this conjecture and show how to predict its value based on the universal critical exponents of the field theory. Analogously, for general $N$ and $D$ we predict the universal critical densities of domain walls and monopoles, for which no detailed thermodynamic study exists. This procedure can also be inverted, producing an algorithm for generating typical defect networks at criticality, in contrast to the canonical procedure [1], which applies only in the unphysical limit of infinite temperature.

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$O(N)$ symmetric scalar field theories are a class of models describing the critical behavior of an great variety of important physical systems. For example, for $N = 3$ they describe ferromagnets, the liquid vapor transition and binary mixtures for $N = 1$ and superfluid $^4He$ and the statistical properties of polymers, for $N = 2$. In the early Universe $N = 2$ describes the phase transition associated with the breakdown of Peccei-Quinn symmetry, and models of high energy particle physics may belong to the universality class of $O(N)$ scalar models, whenever the mass of the Higgs bosons is larger that that of the gauge bosons. $O(N)$ scalar models are also invoked in most implementations of cosmological inflation.

One of the fundamental properties of $O(N)$ $\lambda|\phi|^4$ field theories is the existence, for $N \leq D$, of static non-linear classical solutions, (domain walls, vortices, monopoles) that we will refer to henceforth as topological defects. At sufficiently high temperatures, topological defects can be excited as non-perturbative fluctuations. Their dominance over the thermodynamics, due to their large configurational entropy, is known to trigger the phase transition in $O(2)$ in 3D and 2D, and their persistence at low energies prevents the onset of long range order in $O(2)$ $D \leq 2$ and in $O(1)$ in 1D.

It is therefore natural that the universal critical exponents characterizing the phase transition in terms of defects and through the behavior of field correlators must be connected. This connection is made more quantitative whenever one can construct dual models, field theories which possess these collective solutions as their fundamental excitations [2]. In the absence of supersymmetry rigorous mappings between the fundamental models and their dual counterparts exist only in very special cases [2,3]. Duality has been suggested and empirically observed to be a much more general phenomenon, though.

In this letter we explore the duality between the critical behavior of the 2-point field correlation function and defect densities at criticality. We will show that it leads to the proof that the critical density of vortex strings, observed in recent non-perturbative thermodynamic studies of $O(2)$, is a universal number. Among other insights [4] this shows that the phase transition in $O(2)$ in 3D occurs when a critical density of defects is reached, connecting directly the familiar picture of the Hagedorn transition in vortex densities to the more abstract critical behavior of the fields. We also extend our procedure to different $N$ and $D$, making predictions for the values of the universal densities of domain walls and monopoles, in 2 and 3D.

Finally the inversion of this procedure allows us to easily generate typical field configurations at criticality. This is of fundamental practical importance. Recent experiments in $^3He$ [5] and large scale numerical studies of the theory [6] have lent quantitative support to the ideas, due to Kibble [7] and Zurek [8], that defects form at a second order phase transition due to critical slowing down of the fields response over large length scales, in the vicinity of the critical point. Defect networks hence formed have densities and length distributions set by thermal equilibrium at $T = T_c^+$.

In contrast most realizations of defect networks used, eg., in cosmological studies are generated using the Vachaspati-Vilenkin [1] (VV) algorithm. It relies on laying down random field phases on a lattice and searching for their integer windings along closed paths. The absolute randomness of the phases corresponds to the $T \to \infty$ limit of the theory. More fundamentally it yields defect networks that are quantitatively distinct from those in equilibrium at criticality, i.e., at formation.

Fig. 1 shows the behavior of a system of vortex strings at a second-order phase-transition, for $O(2)$ in 3D. The data was obtained from the study of the non-perturbative thermodynamics of the field theory [9]. At $T_c$ the total density of string $\rho_{\rm tot}$ displays a discontinuity in its derivative, signaling a second order phase transition.

A disorder parameter can be constructed in terms of string quantities by dividing the string population into long string (typically string longer than $\sim L^2$, where $L$ is the size of the computational domain) and loops, comprising of shorter strings. The corresponding densities are denoted by $\rho_{\rm long}$ and $\rho_{\rm loop}$. In Fig. 1 we can observe that $\rho_{\rm long}$ consistently vanishes below $T_c$, except for a small range of $\beta$ where it increases rapidly to a finite critical value. In [9] we conjectured that in the infinite volume limit $\rho_{\rm inf}$ exhibits a discontinuous transition.

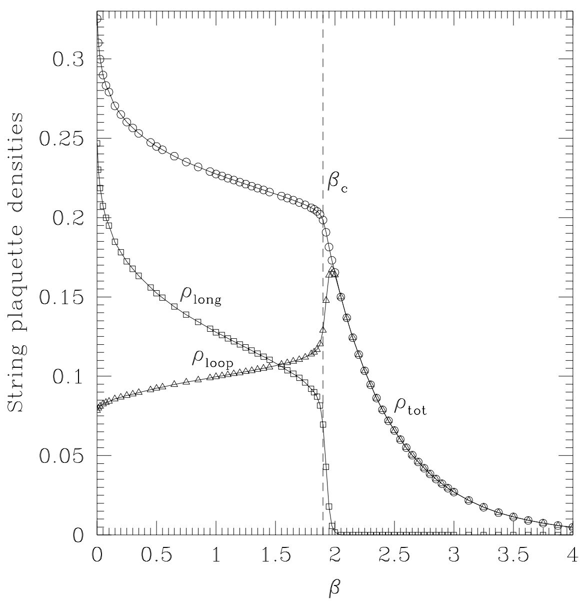


FIG. 1. The string densities, total, loops and long string, as a function of inverse temperature $\beta$. At $\beta_c$, the densities display derivative discontinuities, signaling a second order phase transition. $\rho_{\rm tot}(\beta_c)$ coincides for different studies, leading to the conjecture that it is a universal number.

The value of the total string density at $\beta_c$, $\rho_{\rm tot}(\beta_c) \simeq 0.20$ coincides with results from studies of different models in the same universality class [9,10]. This fact lead us to the conjecture [9] that $\rho_{\rm tot}(\beta_c)$ is universal.

In order to prove this conjecture we appeal to a well known result, due to Halperin and Mazenko [11]. Halperin's formula expresses $\rho_0$, the density of zeros of a Gaussian field distribution in terms of its two-point function. For an $O(N)$ theory the relevant quantity is the $O(N)$ symmetric correlation function $G(x) = \langle \phi(0)\phi(x)^\dagger \rangle$, resulting in

$$\rho_0 \propto \left| \frac{G''(x=0)}{G(x=0)} \right|^{\frac{N}{2}}. \qquad (1)$$

Eq. (1) measures the density of coincident zeros of all $N$ components of the field at a point. Coincident zeros occur at the core of topological defects. Depending on $N$ and $D$, coincident zeros can be interpreted as either monopoles, strings or domain walls. In the particular case of a Gaussian $O(2)$ theory in $D=3$, Halperin's formula allows us to compute the density of vortex strings crossing an arbitrary plane in three dimensional space, a quantity that is clearly proportional to $\rho_{\rm tot}$.

The last key observation is that in the critical domain of a second order transition, all $O(N)$ theories are effectively approximately Gaussian, but with non-trivial critical exponents. In particular renormalization group analysis shows that the mass and quartic coupling vanish at $T_c$ [12,13]. Higher order polynomial terms (eg. $\propto \phi^6$) may be generated but are small. Hence in the critical domain the field two-point function can be written as

$$G(\mathbf{x}) \propto \int d^D\mathbf{k}\, \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|^{-2+\eta}}, \qquad (2)$$

where $\eta << 1.$ is the universal critical exponent taking into account deviations from the mean-field result.

Thus the effective Gaussianity of the theory allows us to use Halperin's result to compute the critical value of $\rho_{\rm tot}(\beta_c)$. Note that, modulo renormalization, the final result depends *only* on $\eta$ establishing, as conjectured, that $\rho_{\rm tot}(\beta_c)$ is a universal quantity.

Substituting, Eq. (2) into (1) we obtain:

$$\rho_{tot} \propto \left(\frac{\eta+1}{\eta+3}\right) \frac{k_{\rm max}^{3+\eta} - k_{\rm min}^{3+\eta}}{k_{\rm max}^{1+\eta} - k_{\rm min}^{1+\eta}}, \qquad (3)$$

where we have introduced upper and lower momentum cut-offs $k_{\rm max}$ and $k_{\rm min}$. In the case of a lattice of size $L$ and lattice spacing $a$ we take $k_{\rm min} = 2\pi/L$ and $k_{\rm max} = 2\pi/a$ which leads to

$$\rho_{tot} \propto \left(\frac{\eta+1}{\eta+3}\right) \frac{1-(a/L)^{3+\eta}}{1-(a/L)^{1+\eta}}. \qquad (4)$$

For large enough lattices, $a/L << 1$, and we obtain

$$\rho_{tot} \propto \left(\frac{\eta+1}{\eta+3}\right). \qquad (5)$$

In order to generate quantitative predictions we need to determine the exact proportionality factor in Eq.(5). This can be achieved by invoking the other instance when the interacting theory becomes Gaussian. In the high temperature limit $\beta \to 0$, the effective interaction becomes irrelevant. In terms of renormalization group the theory displays a (trivial) Gaussian fixed point, with vanishing effective coupling. On the lattice fields at different points will be completely uncorrelated. Note that this situation corresponds to the usual VV algorithm where a field is thrown randomly on the lattice and a network of strings is built by identifying phase windings. Fig. 1 shows the agreement of the densities observed at $\beta = 0.$ with the well known VV result of $\rho_{\rm tot} = 1/3$ with 75% long string. Since the totally uncorrelated field corresponds to a flat power spectrum $G(k) \sim k^0$ we normalize Halperin's expression by imposing $\rho_{\rm tot} = 1/3$ for $\eta = 2$,

$$\rho_{tot} = \frac{5}{9}\left(\frac{\eta+1}{\eta+3}\right). \qquad (6)$$

$\eta$ is always much smaller than 1. Setting $\eta = 0$ we obtain $\rho_{tot}(T_c) = 5/27 = 0.185$, close to the value $\rho_{tot} \simeq 0.2$ observed both in the $\lambda\phi^4$ [9] and $XY$ [10] studies in 3D. A more accurate estimate can be obtained by replacing $\eta$ by its precise value for the universality class to which these theories belong. From [12] we have $\eta \simeq 0.035$ we get $\rho_{\rm tot} = 0.190$, closer to the observed value.

A similar exercise permits the computation of the critical density of domain walls for $O(1)$ and monopoles in a $O(3)$ theory at the critical temperature in 3D.

The density of domain walls per link is

$$\rho_{tot} = \frac{1}{2}\left(\frac{5}{3}\right)^{1/2}\left(\frac{\eta+1}{\eta+3}\right)^{1/2}. \tag{7}$$

Note the value of $\rho_{tot}(\beta = 0) = 1/2$ corresponding to the high-temperature limit. At $\beta_c$ we get, with $\eta = 0.034$ [12], $\rho_{tot}(\beta_c) \simeq 0.38$. For monopoles we will take for the flat-spectrum case $\rho_{tot}(\beta = 0) \simeq 0.1$. A better estimate can be obtained from a tetrahedral discretization of the sphere, resulting in $\rho_{tot}(\beta = 0) = 3/32$ and

$$\rho_{tot} = \frac{3}{32}\left(\frac{5}{3}\right)^{3/2}\left(\frac{\eta+1}{\eta+3}\right)^{3/2}. \tag{8}$$

with $\eta = 0.038$ [12] leading to the critical value $\rho_{tot}(\beta_c) = 0.040$. Finally for domain walls in 2D, the density per link at $\beta_c$ is (using $\rho_{tot}(\beta = 0) = 1/2$):

$$\rho_{tot} = \frac{1}{\sqrt{2}}\left(\frac{\eta}{\eta+2}\right)^{1/2}. \tag{9}$$

Taking $\eta = 0.26$ [12] we obtain $\rho_{tot}(\beta_c) = 0.24$.

The present procedure can be inverted to generate a typical defect network at criticality. The approximate Gaussianity of the field theory at $T_c$ implies that the statistical distribution of fields, $P[\phi]$ is given by

$$P[\phi] = \mathcal{N} e^{-\beta\int d^3k \frac{1}{2}\phi_{-k} G(|k|)\phi_k} \tag{10}$$

This distribution can be sampled by generating fields as

$$\phi_k = R(k)\sqrt{\beta^{-1}G(|k|)} \tag{11}$$

where $R(k)$ is a random number extracted from a Gaussian distribution, with zero mean and unit variance. The field can then be Fourier transformed to coordinate space, its phases identified at each site, and vortices found in the standard way. Since we will be willing to compare results from this algorithm with the ones measured in lattice Langevin simulations we chose to employ the exact form of the field correlator on the lattice:

$$G(|k|)^{-1} = \left[\sum_{i=1}^{D} 2\left(1-\cos(k_i)\right)\right]^{\frac{2-\eta}{2}} \sim_{|k|\to 0} |\mathbf{k}|^{2-\eta}. \tag{12}$$

We have performed several tests on the algorithm, by comparing it to the results of the non-perturbative thermodynamics of the fields at criticality. We used lattices of size $N_{\rm lat}^3$ with $N_{\rm lat} = 16, 32, 64$ and 128. All results are averages over 50 samples obtained from independent random realizations. Fig. 2 shows the string densities for values of $\eta$ between 0. and 0.1, including all reasonable values of $\eta$ in 3D.

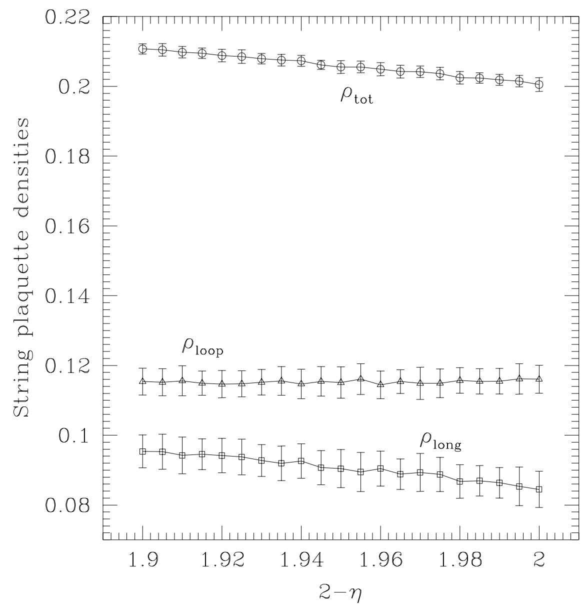


FIG. 2. The string densities from the 50 Gaussian realizations as a function of $\eta$ for a lattice with $N_{\rm lat} = 64$. Error bars indicate standard deviation from the mean.

The values for the densities depend on the size of the lattice, converging to finite values for large $N_{\rm lat}$. In Fig. 3 we can see the scaling of $\rho_{\rm tot}$ with box size for two choices of the critical exponent, the mean field value $\eta = 0.$ and the theoretical result for the $O(2)$ universality class in 3D, $\eta \sim 0.035$. We can predict the form and the power of this scaling through Eq. (4). Writing $a/L = 1/N_{\rm lat}$, the number of points in the lattice, and expanding Eq. (4) in powers of $1/N_{\rm lat}$ we see that Halperin's result converges to its infinite volume limit according to:

$$\rho_{\rm tot}(\infty) - \rho_{\rm tot}(N_{\rm lat}) = \frac{1}{N_{\rm lat}^{1+\eta}} + O(1/N_{\rm lat}^2) \tag{13}$$

To check these scalings we fitted the data of Fig. 3 to a power law of the form:

$$\rho_{\rm tot}(N_{\rm lat}) = \rho_{\rm tot}(\infty) + \frac{A}{N_{\rm lat}^{\alpha}} \tag{14}$$

For $\eta = 0$ and $\eta = 0.035$ we found:

$\eta = 0.0, \quad \rho_{\rm tot}(\infty) = 0.1969, \;\; A = 0.3259, \;\; \alpha = 1.060;$
$\eta = 0.035, \quad \rho_{\rm tot}(\infty) = 0.2012, \;\; A = 0.3422, \;\; \alpha = 1.124.$

These values of $\alpha$ are indeed close to 1, with a larger correction for $\eta = 0.035$ as expected from Eq. (13).

In [9] for a lattice of size $N_{\rm lat} = 100$ we measured $\rho_{\rm tot}(\beta_c) = 0.198 \pm 0.004$. For a Gaussian field with $\eta =$

0.035 we obtain $\rho_{\rm tot} = 0.203 \pm 0.003$. The agreement of the two results is very satisfactory.

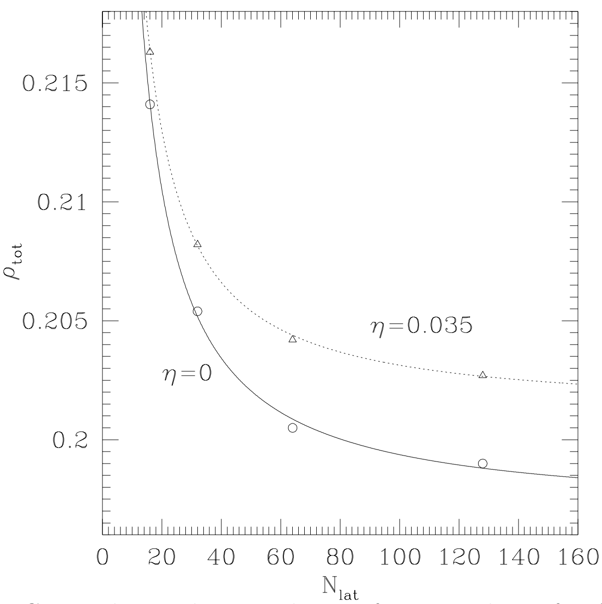


FIG. 3. The total string density for two values of $\eta$ for $N_{\rm lat} = 16, 32, 64$ and 128 and respective fits to a power law. Statistical errors are much larger than the deviation of the points to the fits.

The results for $\rho_{\rm long}$ and $\rho_{\rm loop}$ using these two different methods are also in good agreement. In this case we were not able to find a reasonable scaling expression though, but this is to be expected given the arbitrariness of the long string definition. The results for $N_{\rm lat} = 100$, using $\eta = 0.035$ are $\rho_{\rm long} = 0.080 \pm 0.004$, $\rho_{\rm loop} = 0.121 \pm 0.004$. These compare well with the non-perturbative results $\rho_{\rm long} = 0.076 \pm 0.005$, $\rho_{\rm loop} = 0.120 \pm 0.004$. Even more impressive is that the string length distribution at criticality can also be reproduced by our Gaussian field algorithm. This distribution can be successfully fitted to an expression of the form [9],

$$n(l) = A l^{-\gamma} e^{-\beta \sigma l}. \tag{15}$$

The fit to the results of the Gaussian field algorithm shows a small variation of the parameters $A, \gamma$, and $\sigma$ for $\eta \sim 0. - 0.1$. $\sigma$ is consistently zero, reflecting the fact that the spectrum is always scale invariant. The value of $\gamma$ varies between 2.34 and 2.40. For the critical exponent $\eta = 0.035$ we obtained $\gamma \simeq 2.35$. Once again this is in good agreement with the result from the lattice non-perturbative thermodynamics at $T_c$ [9], $\gamma \simeq 2.36$.

Finally the predictions for $\rho_{\rm tot}$ from Halperin's formula, when compared to the accuracy of the Gaussian algorithm seem rather poor. The expression is meant to apply for continuum distributions, while all other values of $\rho_{\rm tot}$ were obtained on the lattice. A straight substitution of the lattice correlators (12) into (1) increases $\rho_{\rm tot}$ to 0.21 from 0.19, covering our full range of results. To perform a precise comparison however Halperin's formula should be rederived for a field theory on the lattice. Despite these shortcomings Halperin's formula has the merit of being the only analytic way of estimating the critical densities of defects in theories where non-perturbative thermodynamic results are scarce.

We have therefore established the connection between the universal critical exponent characterizing the behavior of the $O(N)$ field 2-point correlator and the critical density of defects. This relation implies that defect densities at $T_c$ for a system undergoing a second order phase transition are universal numbers. We predicted them for several $O(N)$ models in 2 and 3D. Based on these insights we proposed a new algorithm for generating networks of defects at the time of formation. In particular, we have shown that this algorithm reproduces accurately all the features of a string network in 3D at criticality. This procedure, instead of the more usual algorithm of [1] should be used to generate typical defect networks at the time of their formation.

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